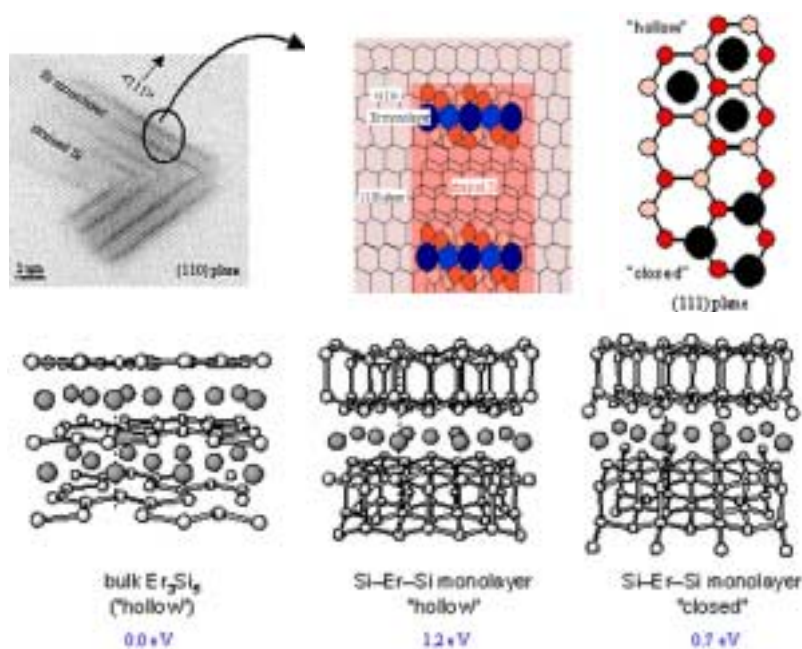


**Structure of Mesotaxial Er Silicide Layers in Si**

P. Citrin, D. Hamann, D. Muller, P. Northrup (Bell Labs) M. de Dood and A. Polman (F.O.M.)  
 Beamline(s): X15B

It has remained a puzzle why, even at low MBE growth temperatures of Si:Er and very low Er concentrations, the Er-Si bond lengths measured by x-ray absorption always resemble those in bulk metallic  $\text{Er}_3\text{Si}_5$ . Scanning transmission electron microscopy data from such dilute alloys has revealed small precipitates, i.e., extended defects, composed of ER monolayers with no Si stacking faults. The absence of stacking faults can occur only if Er atoms occupy “closed” sites in the (111) plane (see Fig. 1), a counter-intuitive configuration because Er occupies “hollow” sites in  $\text{Er}_3\text{Si}_5$ . First principles calculation confirm that the “closed” configuration is indeed the most energetically favored one. The calculations indicate that the stabilization energy originates from Si mediated Er-Er bonding (the Er-Er separation in the Er-Si systems is  $\sim 10\%$  greater than in Er metal). Such bonding in  $\text{Er}_3\text{Si}_5$  is facilitated with Er in hollow sites of the graphitic-like Si planes, but not in bulk Si because the (111) planes are buckled; only in the “closed” configuration is this accomplished. The importance of optimizing Er-Er metal bonding is the key factor in explaining why Er maintains its metal-atom electronic configuration in Si and forms extended rather than soluble point defects.



**Figure 1.** STEM micrograph showing Er monolayers with no Si stacking faults. Schematic pictures show that Er occupies “closed” sites, which are calculated to be energetically preferred over the more conventional “hollow” sites.